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THE BAND-TO-BAND TRANSITIONS IN ZnO and THEIR PRESSURE DEPENDENCE

DR. D. W. LANGER and R. L. KNELL,* Solid State Physics Research Laboratory, ARL

It is generally accepted that compound crystals composed of elements of distinct groups of the periodic table are similar and related by common properties. Examples are the alkali halides, the III-V compounds, and also the IIb-VIa compounds, i.e., the tellurides, selenides and sulfides of mercury, cadmium and zinc as well as zinc oxide, which are all commonly of zinc blende or wurtzite structure. Interband Faraday rotation experiments, e.g., gave evidence that the band-to-band transitions in the II-VI compounds, CdS, CdTe, ZnTe, ZnSe, ZnS, and ZnO are similar, namely direct and allowed. (1) The trend given by the order of the elements in the columns of the periodic table usually is followed by a similar order in the electronic band structure. The band gaps, in the sequence of Cd compounds CdTe, CdSe, and CdS, increase monotonically in the order of increasing ionicity. The band gaps, in the sequence of Zn compounds ZnTe, ZnSe, ZnS and ZnO, also increase in order of increasing ionicity, except for ZnO. The experimental values are roughly 2.2, 2.6, and 3.7, respectively, and 3.3 for ZnO. An estimate based on the trend of the electronegativity given by the other Zn compounds would lead to a value of 4.5 eV for ZnO. This deviation from the trend of the sequence might suggest that the band-to-band transitions of minimal energy in ZnO are not completely analogous in terms of band symmetry or transition point in k-space to those in similar II-VI compounds.

Our measurements reported here for the pressure coefficient of the fundamental absorption edge of ZnO up to 10 kbars at 77^{0}K show a further dissimilarity between ZnO and otherwise similar II-VI compounds.

Paul, sometime ago, drew attention to experimental evidence (2) based on correlations of the pressure coefficients of energy gaps in Group IV and Group III-V compound crystals. He pointed out that, within a given crystal structure, the pressure coefficient of a transition is determined by the symmetry of the bands and of the points in k-space between which the transition occurs rather than by the chemical composition of the crystal or the width of the energy gap. It had been shown that this rule might also apply to II-VI compounds (3).

We measured the pressure coefficients of ZnO and related II-VI compounds. We shall show that, on the basis of Paul's rule, there

* Field Engineer of Malaker Corp.

are further reasons to believe that the fundamental band-to-band transition in ZnO does not occur toward the same type of conduction band or to the same point in k-space as in other II-VI compounds. In our experiments, we are using the reflectivity maxima near 3.385 eV, observable with $E \perp c$, and 3.425 eV, observable in both modes of polarization, at 77°K as indications of the separation of the conduction band with the upper two levels of the valence band. Similar to that of other II-VI compounds of wurtzite structure, the valence band is split threefold due to the spin orbit and crystalline field interaction.

When hydrostatic pressure is applied (the apparatus has been described previously) (4), the shape of the reflectivity structure is largely unchanged, but it is shifted toward higher energies. Figure 1 shows 3 typical measurements out of 53 made between 10 kbars and atmospheric pressure at 77°K. The pressure coefficients, as determined from the values indicated by the dashed lines in Fig. 1, are 2.67 and 2.78×10^{-6} eV/bar ± 2% for the maxima near 3.385 and 3.425 eV, respectively.

The pressure coefficients of the band gaps of II-VI compounds, which have been reported by other authors (5), were mostly obtained through the shift of a constant absorption value as a function of pressure. The middle value of the pressure shift of ZnO, found thusly by Edwards, is 0.6×10^{-6} eV/bar in the pressure range of 1 to 10 kbars. This discrepancy, as compared to our results, might be due mainly to an inability to obtain hydrostatic conditions in this pressure region with his experimental technique. We also feel that the reflection maxima, which coincide with high absorption coefficient values, are a more reliable indication of the absorption edge in II-VI compounds than the normally used comparatively low values of the absorption edge, which might be influenced by

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JACOB SEIDEN
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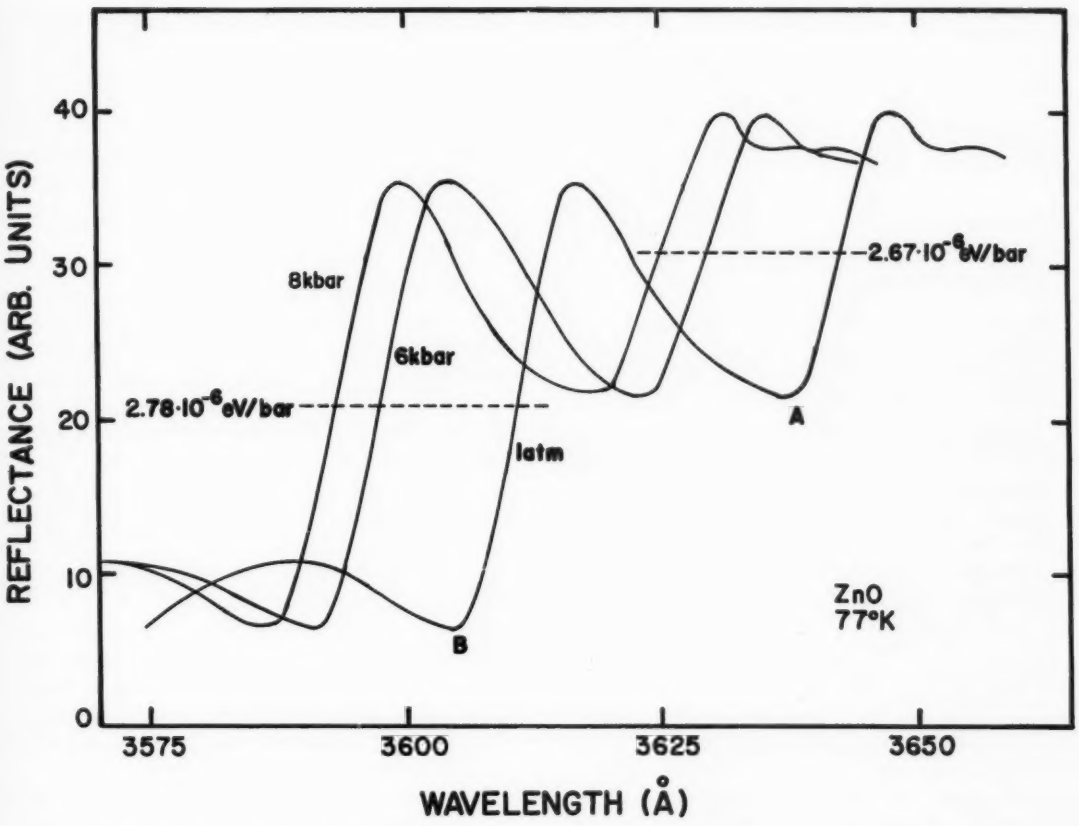

Figure 1. Typical unpolarized reflectance spectra of ZnO at 77°K and various pressures. The coefficients are determined by the intersection with the dashed lines. They are 2.67 meV/kbar for peak A ($E \perp c$) and 2.78 meV/bar for peak B ($E \perp c$ and $E \parallel c$).

impurity or strain broadening.

We determined, similarly, at 77°K and up to 5 kbars, the pressure coefficient of the 1.7 eV maximum in wurtzite CdSe. The pressure coefficients and those of other II-VI compounds, determined previously (3, 6) by the same method, are listed below for comparison with the coefficient of ZnO:

Pressure Coefficients of the Fundamental Band Gap in II-VI Compounds (in 10^{-6} eV/bar)

ZnO	2.7	CdS	4.5	Wurtzite
ZnS	6.3	CdSe	6	Structure
ZnTe	11.3	CdTe	8.0	Zinc blende

ZnTe and CdTe are of zinc-blende structure, and their pressure coefficient is of about the same magnitude as that of transitions of the Γ_1 point of the conduction band in III-V compounds of zinc-blende structure, which is in agreement with Paul's rule. CdS, CdSe, ZnS and ZnO are of wurtzite structure (the ZnS samples were stack-faulted) and should be expected to exhibit, similarly, a common pressure coefficient for conduction-band minima of the same symmetry. The coefficients for CdS, CdSe and ZnS seem to agree fairly well with each other, i.e., within the range of scatter usually observed between different compounds (2). The pressure coefficient of ZnO, however, is remarkably lower than that of the other wurtzite II-VI compounds. On the basis of Paul's rule, this

furnishes independent reasons for the suspicion that a conduction band of different symmetry or transitions to different points in k-space might be involved in the electronic transitions at the fundamental band gap of ZnO. ★

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METALLIC IONS IN THE LOWER IONOSPHERE

UPPER ATMOSPHERE PHYSICS LABORATORY, AFCRL

During meteor showers, metallic atoms from vaporizing meteors are subsequently ionized by the normal photochemical and collisional processes of ionospheric formation. The addition of these ions may greatly alter the composition of the lower ionosphere. In fact, this addition may be correlated with increased sporadic-E activity.* For example, in one series of rocket flights into sporadic-E layers, it was shown that sporadic E was composed entirely of metallic ions.

These are the results and implications of rocket data collected and analyzed by Dr. R. S. Narcisi, A. D. Bailey, and L. Della Lucca of AFCRL. Their investigations were reported in three separate papers presented at the Seventh Annual Space Science Symposium in Vienna, Austria, on 12 and 17 May 1966.

These three papers covered different aspects of two rocket flights that took place on 16 and 17 November 1965 during the annual Leonid meteor shower. The two Nike-Cajun rockets carried unique and highly precise mass spectrometers to sample the composition of the D and lower-E regions of the ionosphere. It is in these regions, which extend from about 50 to 110 km., that atmospheric friction heats and vaporizes meteorites. Metallic ions of meteoric origin were found to make up a sizeable portion of the content of the lower ionosphere.

During the 1965 Leonid shower, Narcisi, Bailey, and Della Lucca found that at altitudes between 85 to 100 km., the positive ions of sodium, magnesium, aluminum, calcium, ion, nickel, and silicon--all substances found in meteorities--constituted 30 to 50 per cent of the total ionization (the remainder being ions of nitric oxide and molecular oxygen). In addition, the AFCRL scientists found that metal-ion concentrations were much lower between 100 and 110 km., the altitude immediately above that at which maximum meteor vaporization occurs.

Data from the 17 November flight, made the night after the shower, also proved significant. On this flight, using a rocket-borne mass spectrometer, sporadic-E layers were sampled--the first time such a feat has been accomplished. The two layers of sporadic E so sampled were found to be composed of the positive ions of iron, magnesium, calcium, and nickel--again, metals found in meteorites.

Although some metallic ions were first detected in the lower ionosphere by other experimenters, the AFCRL scientists were the first to identify the ions of all seven major metals normally found in meteors, and to measure their altitude distributions as well. ★

** Sporadic E is a highly localized layer of increased electron and ion density sometimes a fraction of a km. thick, occurring at unpredictable times, and having a pronounced effect on communications.*

SUNSPOTS & SOLAR ROTATION

The sun rotates once every 27 days--more or less. Actually, the rate varies from about 25 days at the equator to about 31 days at the poles. But at any given latitude, we don't know the exact rotation rate with decimal-point precision because no one has come up with a completely satisfactory way to measure it.

A simple and widely used method of measuring the rotation rate is to observe the movement of sunspots. But the problem is that a given sunspot at a given solar latitude does not necessarily move with the same velocity as another sunspot measured at a later time at the same latitude.

A host of difficulties and uncertainties crop up in the use of sunspots to measure rotation rates. These uncertainties are examined in a recent paper, "The Determination of the Solar Rotation Rate from the Motion of Identifiable Features," by Dr. Fred Ward of AFCRL. In this paper, Dr. Ward reviews the many past studies of others who have attempted to derive solar-rotation rates from sunspot data and re-examines data on sunspot movements going back almost 100 years.

These measurements show that sunspots near the solar equator have an average movement of about 14.5 degrees of longitude each day, while those in the latitude region of 30 to 35 degrees have a relatively slower movement, about 13.7 degrees each day. It is shown, however, that sunspot groups which have long dimensions many times their short dimensions move as much as 2 per cent faster than groups of roughly circular shape; this difference is independent of latitude. Also, small sunspot groups move faster than large groups--this implies that "mature" groups slow down.

The validity of using sunspots as tracers of velocity might be questioned on several points. One factor is that the sunspots are continually exchanging material with their surroundings and, therefore, do not necessarily move with the velocity of the ambient fluid. Since there may be variations in the velocity of this ambient fluid, sunspots may be particularly associated either with fluid in relatively rapid motion or with fluid in relatively slow motion. Still another uncertainty in the use of sunspots as tracers of solar-rotation rates involves the determination of the center of gravity of a sunspot group. During the early stages of formation, this center of gravity shifts counter to the direction of rotation. In the decay stage, the center of gravity shifts in the opposite direction. The center of gravity itself is difficult to compute because it is not always possible to observe very small sunspots within a group, or around its periphery.

After his examination of the many problems in using sunspots as tracers of the sun's rotations, Dr. Ward concludes that the uncertainty in measuring the rotation rate is an order of magnitude larger than previously assumed. This uncertainty is between 0.1 and 0.2 degrees per day. Because of the systematic errors that arise from previous methods of measurement, Dr. Ward proposes that the solar-rotation rate be derived simply from the day-to-day motions of a random selection of sunspot groups. With this relatively simple approach, he finds that the solar-rotation rate is about 1 per cent higher than that arrived at by Newton and Nunn whose calculations of rotation rate are presently the accepted values. ★

waves of ionization in low-pressure gas discharges

DR. A. GARSCADDEN, Plasma Physics Research Laboratory, ARL and
DR. D. A. LEE, Applied Mathematics Research Laboratory, ARL

Electrical discharges in gases at low pressures have been of interest to physicists and others for nearly 200 years. They have provided much of the experimental basis of our knowledge of atomic physics, especially through spectroscopy. Today they are studied with these aspects still in mind, as well as newer interests such as electromagnetic-wave propagation through the gas-discharge plasma, plasma instabilities, the properties of the solar and interplanetary plasmas, and, more recently, gas lasers.

Let us consider a glow discharge in a long cylindrical tube having two plane electrodes at its ends and filled with a pure atomic gas at low pressure (0.5 to 20 torr). The discharge may carry a current in the range of 10 milliamperes for a cathode-anode potential difference of the order of a few hundred volts depending on the length and radius of the tube, the gas used and the cathode material. The discharge regime considered is characterized by a constant voltage across the tube as the current is increased. To an observer this discharge has the appearance shown schematically in Fig. 1. Some bright and dark structures are visible near the cathode end, and there may be irregularities very close to the anode. In their most common pattern, these irregularities are called anode spots. The major portion of the discharge appears to be a homogeneous glow and is referred to as the positive column. This region of the discharge has usually been considered to be an ideal plasma and to be in equilibrium, i.e., the rate of ionization is equal to the losses by ambipolar diffusion and by recombination, and there is only a very small excess positive charge (hence the nomenclature). It is normally assumed that quantities such as the electric field and the ion and electron densities are independent of longitudinal position along the tube.

However, although the positive column of a low-pressure glow discharge may appear visibly homogeneous, very often, when the light emitted is examined with methods capable of time resolution, the light is found to be fluctuating at frequencies in the order of kilocycles. These fluctuations are in the form of waves travelling in the anode-to-cathode direction with velocities typically of

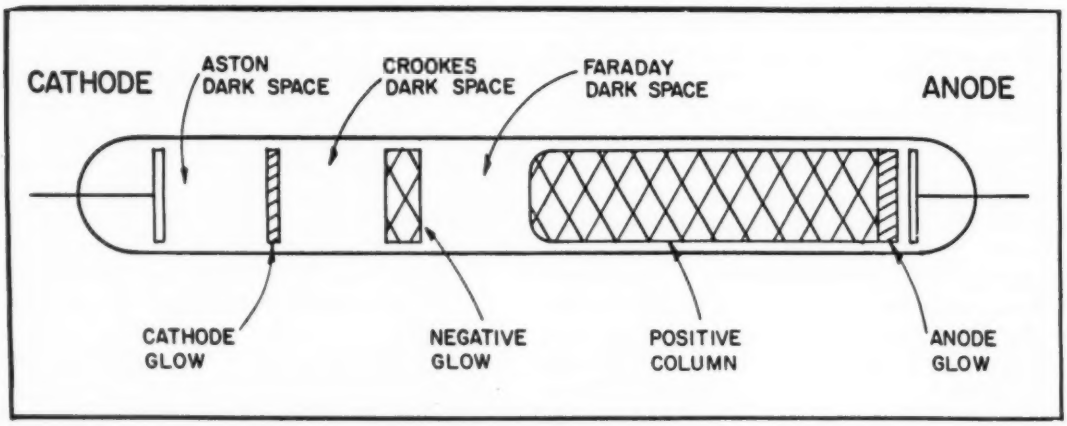

Figure 1. Features of the glow discharge (not to scale).

Figure 2. Smear record of moving striations in a Hg-A low-pressure discharge. Time (ordinate) increases downward. Cathode of discharge is at the left, anode at the right. Phase velocity of the striations is 50 meters/second.

the order of a few hundred meters/second. The intensity fluctuation (amplitude modulation) of the light may approach 100 per cent. Although these waves, termed moving striations, have been known and studied for over a century, it is only in recent years that their description and nature have been put on a quantitative basis.

An intensive study of the phenomenon and its applications has been made in the Plasma Physics Research Laboratory of ARL. The results have been of considerable interest because the ionization waves have been found to have unusual properties, and may occur in gas lasers and influence the laser output. (1)

The moving striations usually occur spontaneously in rare-gas discharges at pressures above 0.5 torr, and exist for moderate currents up to pressures of about 10 torr. There is a high current density cutoff; this has been termed the Pupp limit after the scientist who described it in detail. The diagnostics we used to investigate these waves included smear camera, photomultiplier and spectrographic methods, Langmuir probes and, more recently, image converter techniques. A typical rotating-mirror (or smear camera) record of moving striations in a Hg-Argon glow discharge is shown in Fig. 2. The striations were travelling in the

direction anode to cathode with a velocity of 50 meters/sec. Additional probe and microwave measurements were used to determine the profile of the moving striations in terms of the changes in electron density and electron temperature, as well as in light intensity (Fig. 3). As can be seen, the electron-density variation along the column within a wave length is almost an order of magnitude, and the electron temperature changes by almost a factor of two. Such large variations make the analysis of the phenomenon difficult; for many years the erroneous interpretation was made that, since the striations most often observed travel in the direction anode to cathode, the commonly occurring anode spot oscillations were the source of the moving striations. However, more recently, thanks to an interpretation advanced by L. Pekarek of Czechoslovakia, our understanding of the phenomenon and its effects has improved considerably.

We have been particularly concerned with the dispersion of a pulse applied to a steady nonoscillating positive column because the propagation can be studied under small perturbation conditions. Alternatively, if this condition is not feasible, the study of the development of the glow discharge under pulsed conditions of initiation assists in defining the origin of the instability. A record of this latter experiment is shown in Fig. 4 in which image converter methods were used to obtain spatial and time resolution. The remarkable feature about this instability is that, although the moving striations move in the direction anode to cathode, the wave of disturbance which creates the striations moves in the direction cathode to anode (Fig 4). In other words, these moving striations are an outstanding example of a backward wave, so-called because the phase velocity ($V_p = \omega/\sigma$) and the classical group velocity ($V_G = d\omega/d\sigma$) have opposite directions. (Here $\omega = 2\pi f$ is the angular frequency, $\sigma = 2\pi/\lambda$ is the wave number, λ is the wave length and f is the frequency). We also confirmed this result in other ways, e.g., by frequency pulling an oscillation with an external driving oscillator and directly measuring the dispersion.

The instability has been interpreted by Pekarek as arising from the axial ambipolar diffusion field. This can create a wave of ionization in the following manner. It is possible to show that the ionization frequency at a point in the positive column is a function of the local electron temperature which in turn depends on the local longitudinal electric field. If, because of a noise perturbation, an applied perturbation, or an electrode instability, etc., there is an increase in plasma density over a small region, after a very short time an axial ambipolar space charge field will be created at its edges due to the density gradients. To the anode side, this additional field will act in the opposite direc-

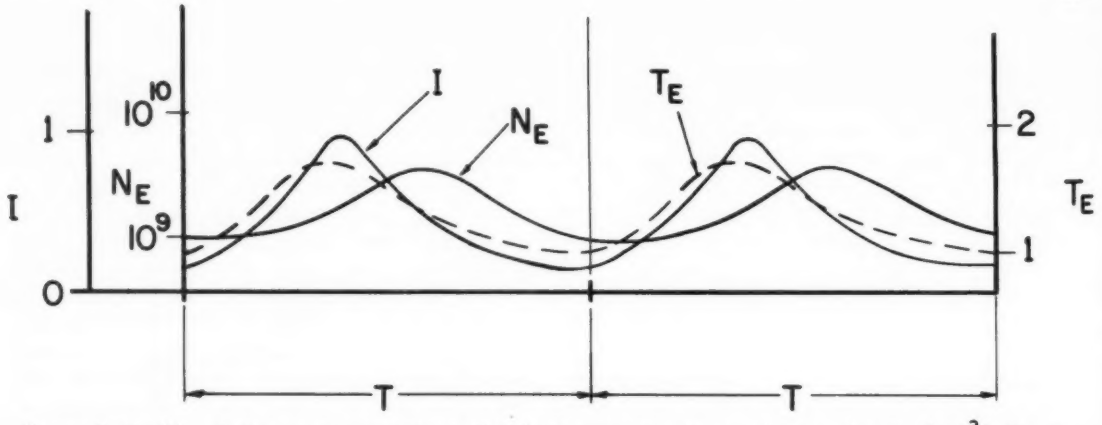

Figure 3. Profile of the moving striations. I is light intensity, N_E is electron density (cm^{-3}), T_E is electron temperature (electron volts), T is period of one wave.

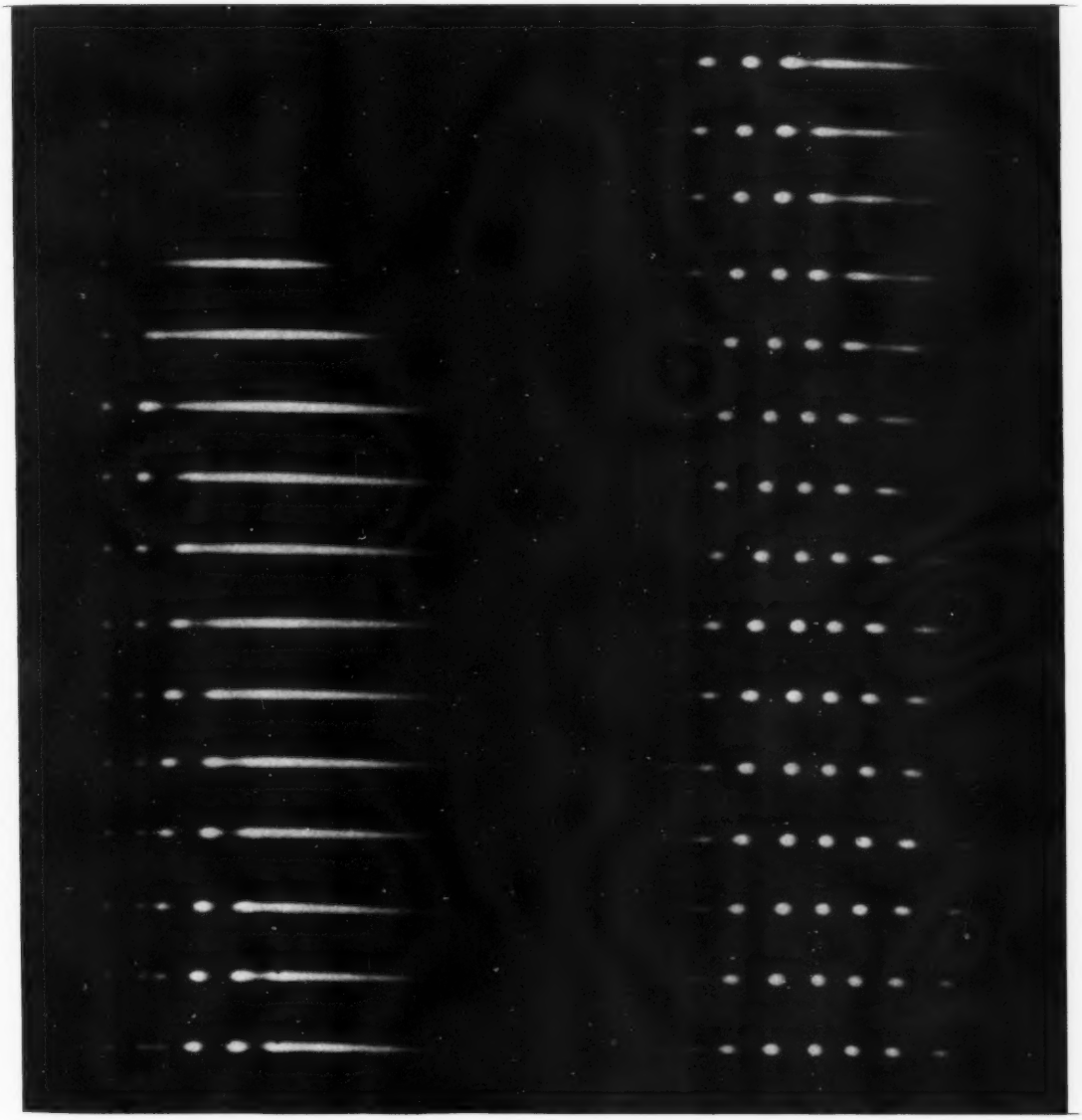

Figure 4. Image converter records of the initiation of a glow discharge. The exposure time of each of the 30 frames is 1 microsecond. The first frame (at the top left) is at switch-on; then there is a 1.05 millisecond delay between the first and third frames (advancing downward). Subsequent frames are at 100 microsecond intervals.

tion to the discharge electric field. This will then reduce the electron density to the anode side of the original disturbance. However, this region of reduced electron density will create an axial ambipolar space charge field to its anode side which will add to the discharge electric field and thus create a new region with increased electron density. Thus, by this mechanism the disturbance propagates.

Our experimental results have been compared with the results of calculations derived

from a solution of equations using the above model. Rather good agreement has been obtained. (2) The onset of the instability, its frequency, wave length and velocities are all obtainable from the basic parameters of the discharge (gas pressure, electric field, electron temperature, and the electron ionizing efficiency for the gas utilized). The theory gives the dispersion relation shown in Fig. 5. Recently, at higher pressures, we have found a type of moving striations which appears to correspond to the forward wave branch of the diagram. We have observed that these oscillations are associated with the onset of radial constriction in the discharge, the direction of the onset of the constriction being in the direction of the group velocity of the striations. We are continuing our studies to describe experimentally and theoretically the onset of the striations as there appears to be a causal relationship between the onset of the constriction and the high-pressure band of moving striations. ★

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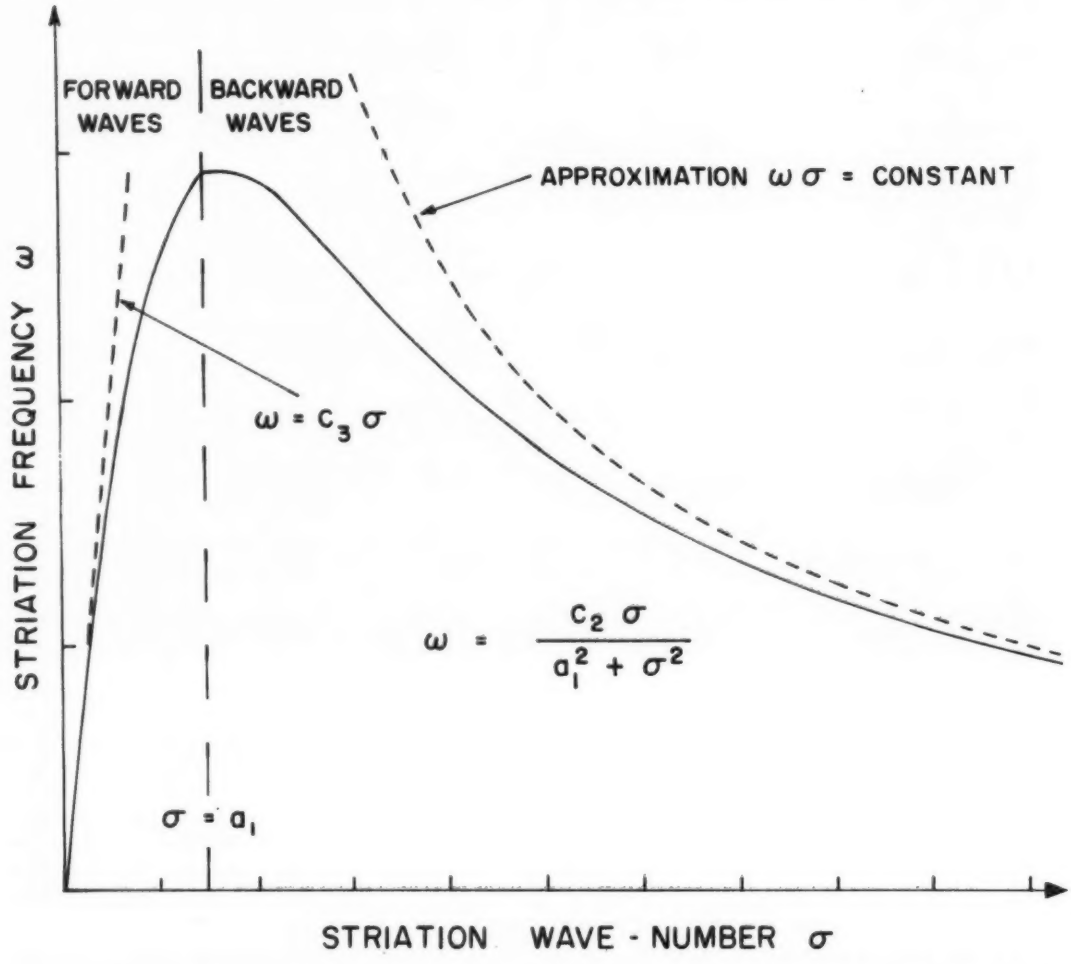
FORWARD WAVES
BACKWARD WAVES
APPROXIMATION ω σ = CONSTANT
ω = C3 σ
ω = C2 σ / (a1^2 + σ^2)
σ = a1
STRIATION FREQUENCY ω
STRIATION WAVE - NUMBER σ

Figure 5. Dispersion relation for moving striations. (Notations are defined in Reference 2.)

CONTROL OF UNSTABLE MECHANICAL SYSTEMS

CAPT JOHN F. SCHAEFER
Aerospace Mechanics Division, FJSRL

Unstable mechanical systems constitute a class of dynamical systems which have been of increasing interest to control-theory engineers over the past decade. The most noteworthy example of such a system is a steerable rocket vehicle during its launch phase. Aerodynamically unstable at low speeds, such a vehicle requires a sophisticated control mechanism to insure that it follows the desired trajectory. The present tempo of successful launches and missions indicates that sufficiently sophisticated controllers have been designed for today's vehicles; but it is not clear that contemporary techniques will suffice for the future.

For example, the continuing stress on maximizing the payload/booster mass ratio indicates that future missiles may be significantly more flexible than those presently in use. This eventuality would seriously compound the controller problem, for then the guidance system must not only maintain vehicle attitude and adherence to the desired track, but must also control the complex interbody motions allowed by flexibility.

A study (1) was made of the effects and ramifications of extreme flexibility of a relatively simple unstable mechanical system on the control and controllability of that system. In this study, the device shown in Figure 1 was constructed and operated for extended times. The model consists of a motor-driven cart to which is hinged a highly flexible beam. The cart motor is controlled so as to drive the cart horizontally and thus balance the beam vertically. Such a device is inherently unstable and imposes controller requirements quite similar to those generated by the flexible booster discussed above.

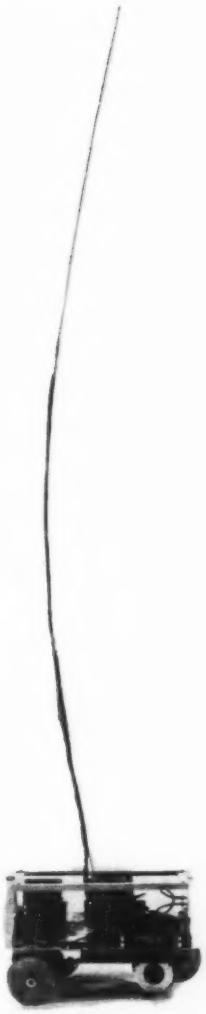

Figure 1. Limber Beam Controlled Experimentally

This experimental study, conducted at the Aerospace Mechanics Division, FJSRL, yielded several significant results. Among them was the realization that a control thruster (cart motor) of limited output could not only balance the beam, starting from sufficiently small initial conditions, but could also dampen motions due to an arbitrary number of the beam's bending modes. Systematic

techniques for synthesizing a feedback-control law to actively control any number of such modes were developed.

A portion of the analysis was devoted to a study of the behavior of the experimental system as the beam's structural stiffness was (mathematically) varied. It was found that, at certain low values of structural rigidity, the assembly could not be controlled, regardless of the horizontally directed thrust levels available. This result is readily extendible to the problem of controlling the bending motions of a flexible missile, and indicates that certain combinations of structural stiffness and longitudinal accelerations must be avoided if lateral stability is to be achieved by thrust-engine gimballing alone. ★

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ELECTRON-PARAMAGNETIC-RESONANCE STUDIES IN THREE CRYSTALLINE FORMS OF CADMIUM SULFIDE

DONALD R. LOCKER
Solid State Physics Research Laboratory
ARL

In a previous issue of the OAR Research Review (Vol IV, No. 5, Jul 65), a phenomenological description was given of Electron Paramagnetic Resonance (EPR) of centers in diamagnetic host materials. As stated before, the EPR spectrum of some paramagnetic ion contained in a crystal lattice is, in many cases, quite sensitive to the symmetry of the electric fields about it. Because of this, a large number of studies have been made in years past of parameters involved in going from one material to another with the same paramagnetic impurity, or from one impurity to another with the same material. Only in a few cases has one been able to keep the same material and alter the symmetry. Thanks to the work of Gale and Kulp (1) of our Laboratory, it is now possible to study a paramagnetic ion in as many as three different symmetries of cadmium sulfide. Ordinarily, cadmium sulfide is available only in its hexagonal crystal form called Wurtzite. However, by a hydrostatic compression to about 30,000 atmospheres, it may be largely converted to the cubic form of ordinary table salt. Usually, when the pressure is removed, the structure undergoes a change to another cubic form called zinc blende. At this point, Kulp made a real contribution by correctly surmising that, if the pressure vessel could be constructed so that it could be cooled in liquid nitrogen before the pressure was released, the second phase change might be stopped and the "table-salt" phase made available for observations at ambient pressure. Now, by starting with cadmium sulfide doped with various paramagnetic ions, one can observe these ions in three crystalline forms without changing to another compound.

Figure 1 shows a section of the pressure bomb used by Gale and Kulp to produce the transition. The sample is placed in the center, sandwiched between two cleaved discs of rock salt. When the two pistons are forced in by a hydraulic press, the salt flows, by plastic deformation, to achieve a somewhat hydrostatic pressure in the region of the sample. After cooling in liquid nitrogen, the pressure is released, the bomb disassembled, and the sample removed while still immersed. The sample is then transferred in a small vessel of liquid nitrogen to the Dewar of an electron-paramagnetic-resonance spectrometer. If the sample contains manganese, one observes the spectrum of Figure 2. The spectrum is given at two microwave powers to show that these are really two manganese spectra involved. If the sample is allowed to warm up to room temperature and recooled, one gets the spectrum presented in Figure 3. This represents only one manganese spectrum, and is associated with the remain-

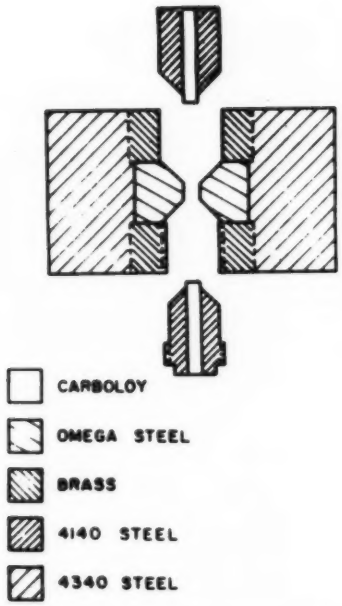

Figure 1. A section of the pressure bomb used to produce the phase transition

ing zinc-blende structure. The one which has disappeared was that due to the "table-salt" phase which is not stable at room temperature. Six major lines are present in a Mn^{++} spectrum due to the six possible orientations of the nucleus. Usually, as is true in the case of Mn^{++}, the interaction between the electron spin and the nuclear spin is greater when the crystal is more ionic in character. In this example, the more ionic situation of the "table-salt" form of cadmium sulfide has given the expected larger interaction, which is manifested in a larger splitting for the six lines. The other smaller lines are the result of electron flips accompanied by nuclear flips. These transitions are forbidden and do not occur in the high symmetry of the "table-salt" phase.

The work described here for manganese-doped cadmium sulfide has been expanded at ARL. Currently, work has been done on the paramagnetic ions, chromium, and vanadium at liquid-nitrogen and liquid-helium temperatures. ★

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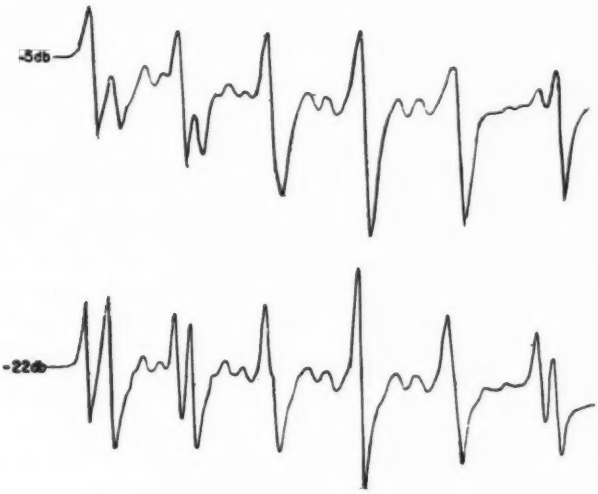


Figure 2. CdS:Mn^{++}
Sample as removed from bomb
Spectrum at 77°K
500 Gauss at 3270 mc

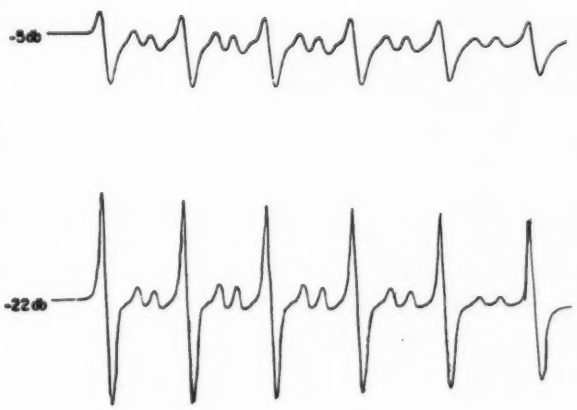
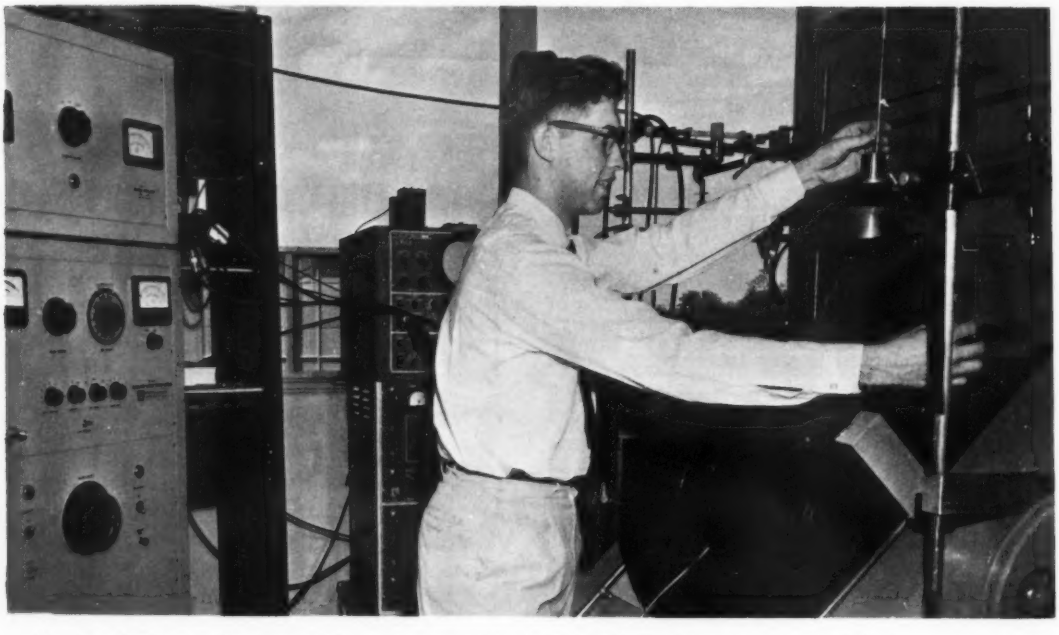


Figure 3. CdS:Mn^{++}
Sample after anneal at room temperature
Spectrum at 77°K
500 Gauss at about 3270 mc

PROFILES

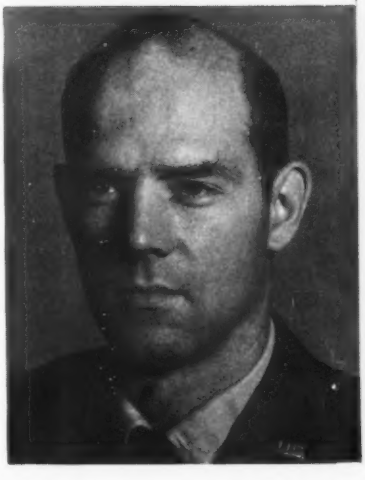
Dr. Dietrich Langer, senior physicist, Solid State Physics Research Laboratory, has been with ARL since September 1957. As leader of a group concerned with pressure effects in semiconductors, he is responsible for giving broad general direction to the research in that field. Dr. Langer attended the Technische Universität in Berlin where he received the "Diplom-Ingenieur" degree in 1957. Under the "paperclip" program, he then immigrated into the United States, later to join ARL. Having completed the necessary course work leading to the Ph.D. at Berlin, Dr. Langer worked on his thesis while at ARL and, in December 1960, received his doctorate at the Technische Universität of Berlin.

Dr. Langer is a member of the American Physical Society and is well known to the national and international scientific community for his work. He is author or coauthor of some 20 technical reports and journal articles in his field. In this issue of the Review, he discusses "Band-to-Band Transitions in ZnO and Their Pressure Dependence."



Mr. Donald R. Locker, an ARL scientist with the Solid State Physics Research Laboratory, is currently working on Electron Paramagnetic Resonance. He has perfected electron-paramagnetic-resonance equipment with superior characteristics, and is using this with a new electron-bombardment cavity to assess radiation-damage centers in ZnSe. Mr. Locker has a B.S. and M.S. (1960), both from the University of Washington. He has several publications to his credit. He writes in this issue of the Review on "Electron-Paramagnetic-Resonance Studies in Three Crystalline Forms of Cadmium Sulfide."

Captain John F. Schaefer was assigned to the Aerospace Mechanics Division, Frank J. Seiler Research Laboratory, in March 1965. Prior to this assignment, he attended Stanford University where he received the Ph.D. degree in Electrical Engineering (1965). Captain Schaefer is a member of the Institute of Electrical and Electronic Engineers, and is the author of the article, "Control of Unstable Mechanical Systems," which appears in this issue of the OAR Research Review.



Captain Lawrence J. Schroeder, a member of the hypersonics group at ARL, is currently investigating the optimization of reentry lifting bodies. In this connection, a computer program has been developed which has produced solutions of optimal lifting bodies. In addition, an experimental study is being planned to determine the aerodynamic characteristics of these configurations in the ARL hypersonic wind tunnels. Captain Schroeder obtained his B.S. (Aerospace Engineering) from Iowa State University, 1956, and his M.S. (Aerospace Engineering) from the University of Oklahoma, 1964. His experience includes: aerodynamicist, McDonnell Aircraft Corporation (1956-1957); student, University of Oklahoma, AFIT-CIP (1962-1964); and engineer, Hypersonic Research Laboratory, ARL, from 1964 to the present. Captain Schroeder joins Dr. W. L. Hankey in discussing "Optimization of Hypersonic Lifting Bodies" in this issue of the Review.

Dr. Rollin E. Hook, a scientist with the Metallurgy and Ceramics Research Laboratory, ARL, writes in this Review on "The Role of Elastic Anisotropy in Bicrystal Deformation." He has a B.Sc. in Metallurgical Engineering from Purdue University, West Lafayette, Indiana (1956), an M. S. in Metallurgical Engineering (1959) and a Ph.D. in Metallurgical Engineering (1966), both from O.S.U., Wright-Patterson AFB, Ohio. From 1956 to 1957, he was employed as a metallurgist with the Dow Chemical Research Laboratory, and from 1957 to 1960 served as a 1st Lt in the USAF. He is a member of several professional societies, and received the Outstanding Achievement Award for 1962, Dayton Area National Engineers Week.

Dr. David A. Lee is currently working on a statistical theory of inhomogeneous turbulence. He is investigating properties of the second-order two-point velocity correlation tensor in steady, inhomogeneous turbulence, with particular attention to the ultimate decay of eddy energy in a stratified turbulence. Dr. Lee received his Ph.D. (Mechanics) from the Illinois Institute of Technology (1963), his Sc. M. (Applied Mathematics) from Brown University (1961), and his B.S. (Electrical Engineering) from the University of Missouri (1950). He was an engineer with Westinghouse Electric Corp., Baltimore, prior to joining ARL as a research mathematician and an officer on active duty. He is now in civilian status. Dr. Lee is coauthor with Dr. Garscadden of the article, "Waves of Ionization in Low-Pressure Gas Discharges," which appears in this issue of the Review.

Dr. Alan Garscadden is currently concerned with the investigation of departures from equilibrium, in particular of oscillations and transients in low-pressure, low-energy discharges. He received his Ph.D. in Physics (1961) and his B.S. (Honours) in Physics (1958), both from Queen's University of Belfast, Ireland. Since February 1962, he has been a research physicist in ARL's Plasma Physics Research Laboratory. Prior to then, he served as a research assistant to Professor K. G. Emeleus, Queen's University of Belfast, working on plasma radiation and plasma oscillations. Dr. Garscadden has written numerous papers. In this issue of the Review, he and Dr. D. A. Lee discuss "Waves of Ionization in Low-Pressure Gas Discharges."

Dr. Wilbur L. Hankey, Senior Aerodynamicist with the Hypersonic Research Laboratory, ARL, conducts basic research in the general field of fluid motion, emphasizing hypersonic investigations. As Research Group Leader, he supervises the technical effort of several aerospace engineers conducting analytical and experimental hypersonic investigations. This includes hypersonic pressure distributions, skin friction, heat transfer, and flight mechanics associated with re-entry configurations. Dr. Hankey received his Ph.D. (Aeronautical and Astronautical Engineering) from Ohio State University, 1962; his M.S. (Engineering) from the Massachusetts Institute of Technology, 1953; and his B.S. (Engineering) from Pennsylvania State University, 1951. He has received two ASD awards for the "Most Distinguished Engineering Paper," one in 1962, and the other in 1963. In this issue of the Review, Dr. Hankey and Captain L. J. Schroeder describe "Optimization of Hypersonic Lifting Bodies."

OPTIMIZATION OF HYPERSONIC LIFTING BODIES

DR. WILBUR L. HANKEY and
CAPT LAWRENCE J. SCHROEDER
Hypersonic Research Laboratory, ARL

The first successful recovery of objects from space has been achieved by means of ballistic devices. This pure drag scheme offers the simplest and most efficient method of re-entry; however, the recovery site is restricted to lie in the orbital plane since no ability to produce lateral range exists. In order to attain lateral maneuverability during re-entry to permit recovery of spacecraft at some preselected landing site, one is led to investigate lifting as well as drag re-entry. The USAF and NASA have been developing the technology for lifting vehicles for several years. One of these investigations is being conducted in the Hypersonic Research Laboratory at ARL. This study is concerned with the optimization of lifting configurations. The objective is to determine the vehicle shape that will produce maximum hypersonic lift-to-drag ratio, L/D, (which then produces maximum lateral range) for various physical constraints.

Classically, the mathematical technique designed to solve such problems is the calculus of variations. This technique is quite restrictive, however, and its use has provided only limited success for this particular problem. The use of crude numerical techniques on elaborate digital computers has proved much more successful. A generalized surface with a finite number of geometric degrees of freedom (for example 16) was programmed for the IBM 7094.

Equations were written in terms of geometric quantities to constrain parameters such as volume, surface area, skin friction, aerodynamic heating rate, stability, etc. A technique was developed for systematically examining each degree of geometric freedom to ascertain the optimum value which would produce maximum hypersonic L/D for any combination of constraints. (1) Some of the results will be presented here.

The primary mission of a lifting body is to enclose a prescribed payload (volume requirement) with minimum structural weight (wetted-area limitation) and produce the highest possible hypersonic L/D. A geometric quantity which represents this payload-to-structural-weight ratio is volumetric efficiency (η). This is a dimensionless ratio of a volume-area parameter referenced to a sphere.

$$\eta = \frac{\forall\, 6\sqrt{\pi}}{A_W^{3/2}}$$

A sphere then possesses an η of unity and all other closed geometric shapes have values less than one (unfortunately, a sphere possesses an L/D of zero). Upon command to maximize hypersonic L/D with only a constraint of volumetric efficiency, the computer, after some struggling, produced configurations of the type shown in Figure 1. This body possesses a sharp wedge-shaped nose that evolves into a conical shape with a hemispherical base. This configuration must be viewed as a classical shape with minimum constraints since, for example, it obviously cannot survive heating. It serves as a goal which a practical vehicle can only approach in the limit. Application of a heating constraint along with the command to again maximize L/D for a prescribed volumetric efficiency produced a similar configuration with the addition of a blunted leading edge. The performance characteristics of this configuration are shown in Figure 2. Hypersonic L/D is plotted versus the heating-rate material limit of the nose. Note that for a heat-

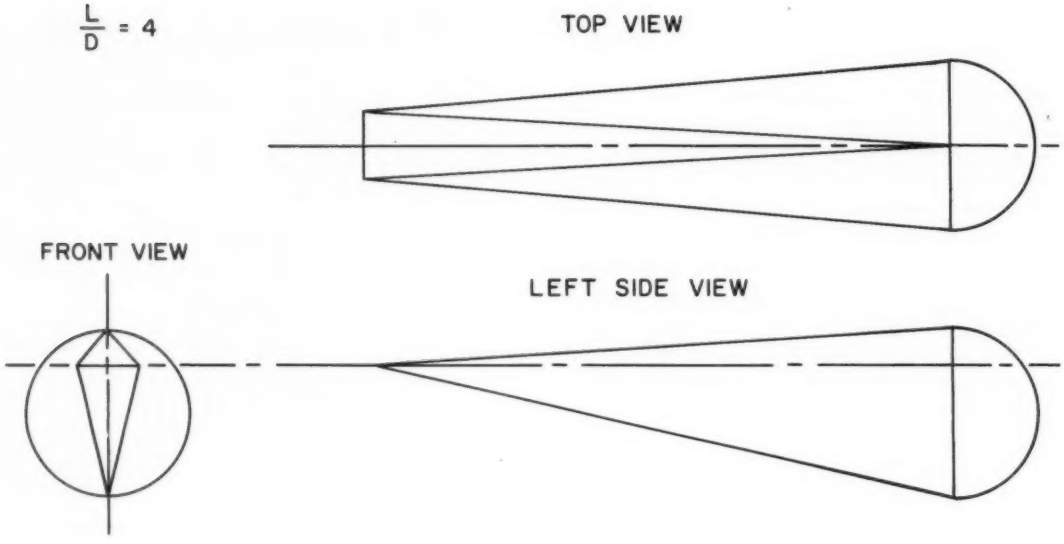


Fig. 1. Typical Optimized Lifting Body

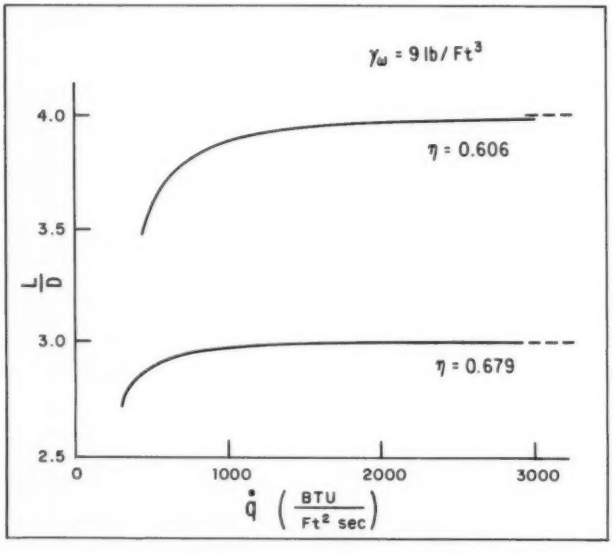


Fig. 2. Heating Constraint Influence on L/D

ing rate of about 1,000 Btu/ft^2 sec the classical optimum is essentially attained. Unfortunately, the present state-of-the-art for nonablative nose caps is about 200 Btu/ft^2 sec. However, one can anticipate material improvements in the future which someday can essentially render the heating constraint negligible in hypersonic vehicle design.

Work is continuing in the investigation of the influence of additional constraints on the characteristics of lifting configurations. ★

REFERENCE

(1) Hankey, W. L. and Capt. L. J. Schroeder, "Optimization of Lifting Re-Entry Bodies," 12th Annual Air Force Science and Engineering Symposium, Vol. 1, 1965.

THE ROLE OF ELASTIC ANISOTROPY IN BICRYSTAL DEFORMATION

DR. ROLLIN E. HOOK
Metallurgy and Ceramics Research Laboratory, ARL

The research program on the deformation of bicrystals was discussed in the October 1965 OAR Research Review. This research has now come to a conclusion. One interesting aspect of the results of this work concerns the importance of elastic anisotropy.

Three isoaxial-type bicrystals investigated, produced by the diffusion bonding of single crystals of an Fe-3% Si alloy, are shown in Figure 1. Each of the six component single crystals has an identical axial orientation (the Z axis), and each is oriented for single slip on a $\langle 111 \rangle$ $\{110\}$ primary slip system, i.e., a $\{110\}$-type crystallographic plane is oriented at 45° with respect to the Z axis, and a $\langle 111 \rangle$ slip direction in this plane is oriented at 45° with respect to the Z axis. The symmetric bicrystal, Figure 1a, is crystallographically symmetric with respect to the XZ grain boundary plane, that is, the

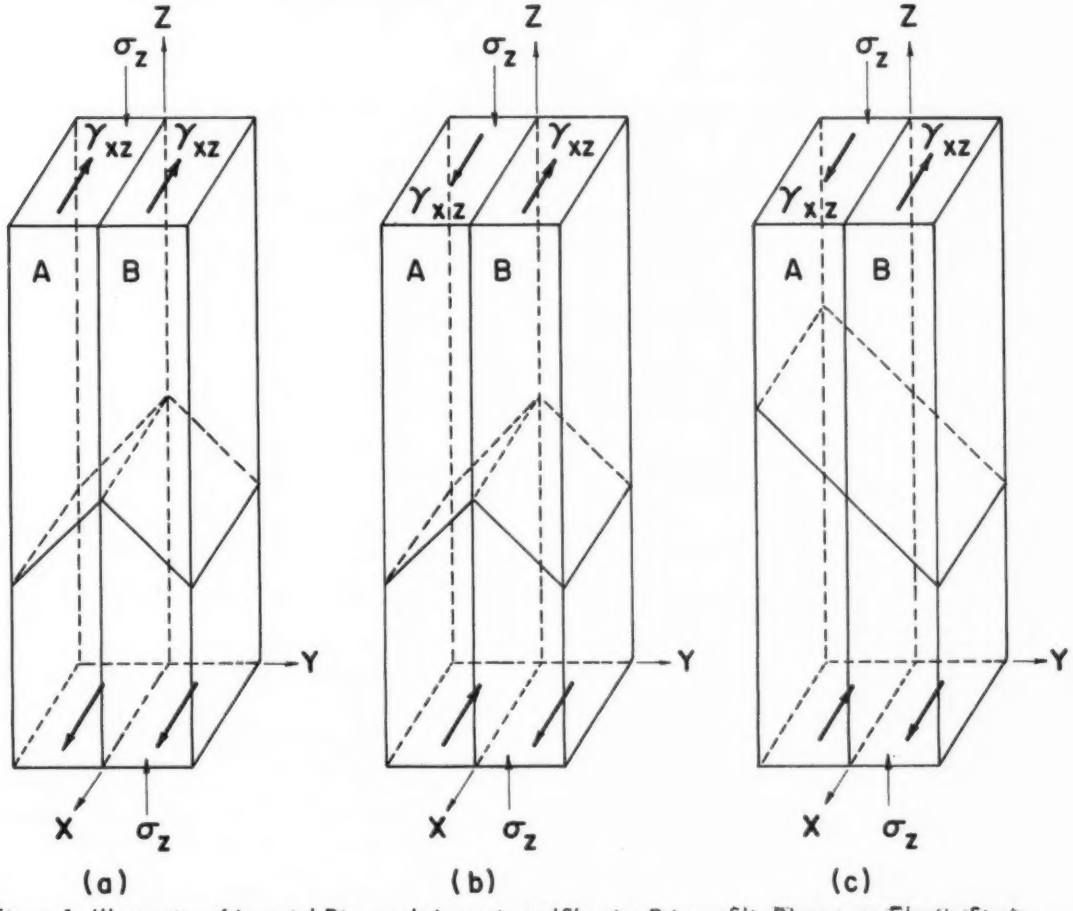


Figure 1. Illustration of Isoaxial Bicrystals Investigated Showing Primary Slip Planes and Elastic Strain Compatibility Due to Anisotropy: (a) Symmetric Case, (b) Pseudosymmetric Case, (c) Pseudoidentical Case.

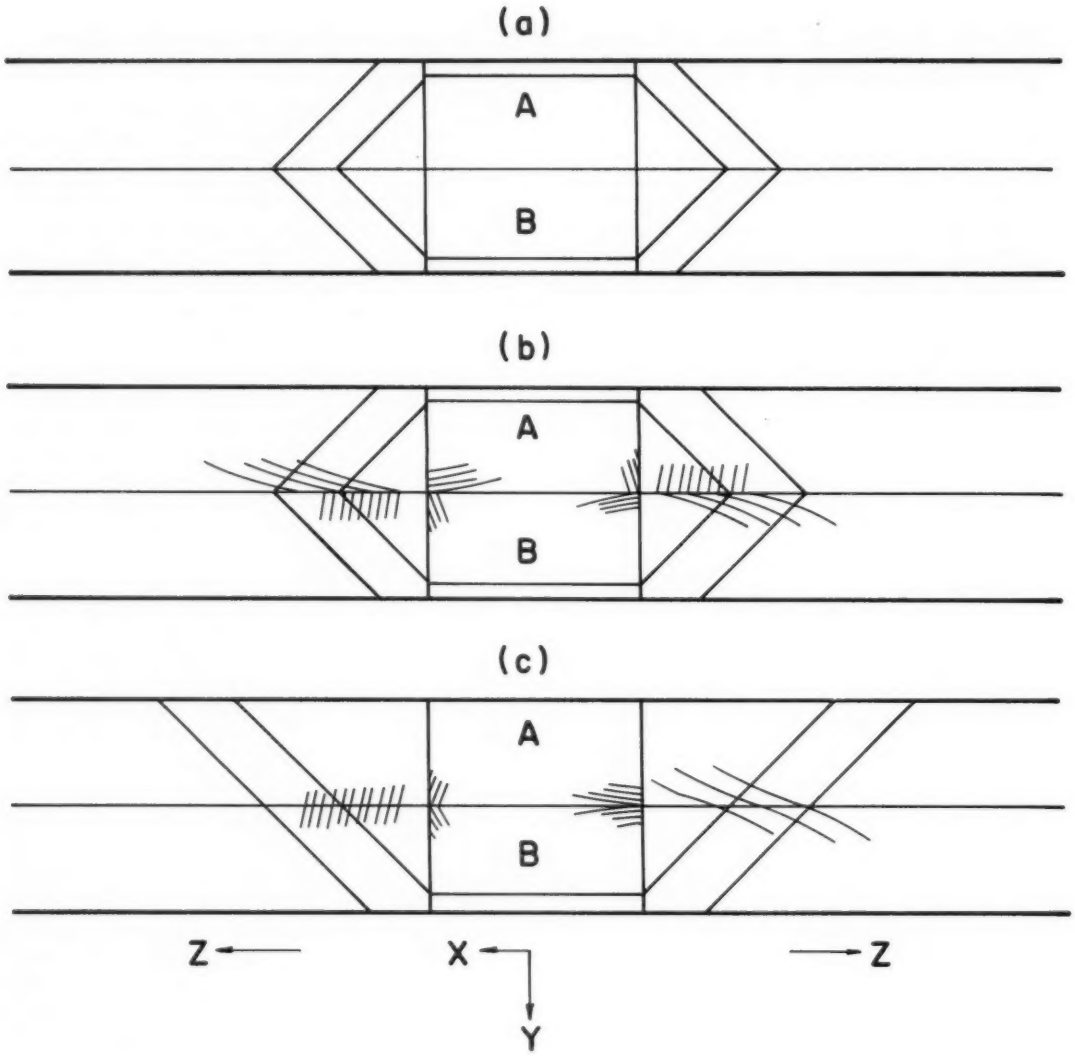


Figure 2. Schematic Illustration of Operative Slip: (a) Symmetric Case, (b) Pseudosymmetric Case, (c) Pseudoidentical Case.

crystal lattices are mirror images across this plane. For the pseudosymmetric bicrystal, Figure 1b, the $\langle 111 \rangle$ $\{110\}$ primary slip systems in each component crystal are symmetric with respect to the grain boundary plane, but the crystal lattices are not. For the pseudoidentical bicrystal, Figure 1c, the primary slip system in one component crystal is continuous with the primary slip system in the other component.

When each of the bicrystals is subjected to a compressive stress, σ_z, the elastic strain components ϵ_x, ϵ_y, ϵ_z, γ_{yz}, γ_{xz}, γ_{xy} which result in response to the application of this simple stress state can be calculated from anisotropic linear elasticity theory. The strain components of importance regarding deformation of the XZ grain boundary plane are ϵ_x, ϵ_z, and γ_{xz}. These elastic strains must be equal for the A and B component crystals of a bicrystal if they are to be elastically compatible. The results of the

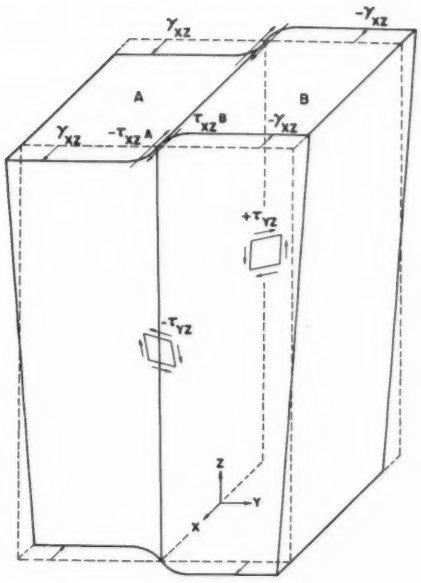


Figure 3. Schematic Illustration Showing Stresses Arising Due to Elastic Incompatibility γ_{xz}.

elastic strain calculation show that the γ_{xz}'s are of considerable magnitude and, furthermore, that these strain components are compatible for the symmetric case but are not compatible for the other two cases, as indicated in Figure 1a-c.

Each of these bicrystals is plastically compatible; that is, plastic deformation can occur solely by slip on the primary slip system in each component crystal since the resulting plastic strain components ϵ_x, ϵ_z, γ_{xz} are equal for both component crystals in each bicrystal. There is no requirement for the operation of additional slip systems in the vicinity of the grain boundary plane in order to satisfy plastic deformation compatibility requirements.

Each of the bicrystals were deformed in compression to a plastic strain of about 0.001. The slip that occurred was then examined by a dislocation etch-pitting technique following an annealing treatment at 160°C for 1 hour which allowed carbon impurity atoms in the alloy to segregate to the slip dislocations, rendering them as preferred sites for formation of etch pits during electrolytic etching of the sample. The slip which occurred is shown schematically in Figure 2a-c.

Slip occurred in the symmetric bicrystal on the primary slip system in each component crystal. The bulk slip behavior of the other two bicrystals was also characterized by single slip on the primary system in each component but, in addition, secondary slip occurred at the grain boundary at and near the lateral bicrystal faces as shown in Figure 2b and c. This secondary slip was homogeneously distributed along the entire length of boundary on the lateral bicrystal surfaces and occurred on slip systems on which the applied resolved shear stress alone was insufficient to cause this slip. This secondary slip is satisfactorily explained in terms of a self-stressed condition arising from the elastic incompatibility in γ_{xz}. This kind of incompatibility results in a twisting of the bicrystal about the Z axis as it is elastically compressed along the Z axis. This leads to the development of shear stresses $\pm \tau_{yz}$ which are at a maximum at the grain boundary at the lateral bicrystal surfaces, Figure 3. These additional stresses assist the applied stress in causing plastic deformation to occur on the observed secondary-slip systems. An analysis of the way in which the stresses $\pm \tau_{yz}$ are resolved onto all the possible slip systems for these two bicrystals is consistent with the secondary slip actually observed. ★

METEOROLOGY LABORATORY, AFCRL

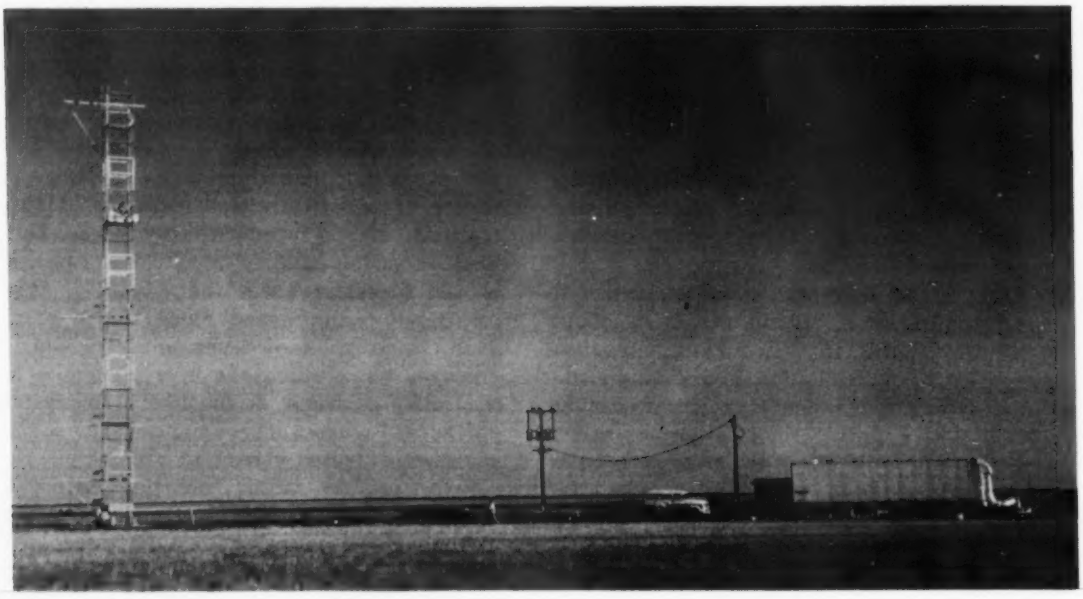
project "WINDY ACRES"

This fall AFCRL meteorologists will again carry out a series of microscale meteorological observations under their "Windy Acres" program. This program was started in the summer of 1965 to investigate the structure and properties of turbulence in the first 100 feet of the atmosphere. The experiments last year were conducted in southwestern Kansas in a flat, level wheat field where natural turbulence can be measured without interference from trees, buildings, and terrain irregularities. The program uses a computer-controlled data-acquisition system for rapid handling and processing of data from various micrometeorological sensors at the field site. This system, called the Mobile Micrometeorological Observation System (MMOS), was developed by AFCRL scientists.

Phenomena occurring in the first hundred feet of the atmosphere are of considerable importance to micrometeorologists. It is here that heat and water vapor are transferred between the earth and the atmosphere. These processes can be understood best by examining air turbulences near the ground.

A large body of information is available on turbulence in wind tunnels, but not so much on turbulence in the real atmosphere. Studies in the atmosphere are complicated not only by the existence of a wide range of eddy sizes, but also by a wide range of temperature variations in space and time. The most fruitful approach to this problem is the application of statistical concepts developed in the fields of fluid mechanics and aerodynamics. A detailed systematic study of this type involves the recording, processing, and analyzing of enormous volumes of experimental data.

Experimental field programs in the past have been hampered by the inability to handle large amounts of data in the field. This difficulty however, is now overcome through the use of MMOS, which automatically con-



View of experimental site in Kansas

trols all the operations required in an experiment.

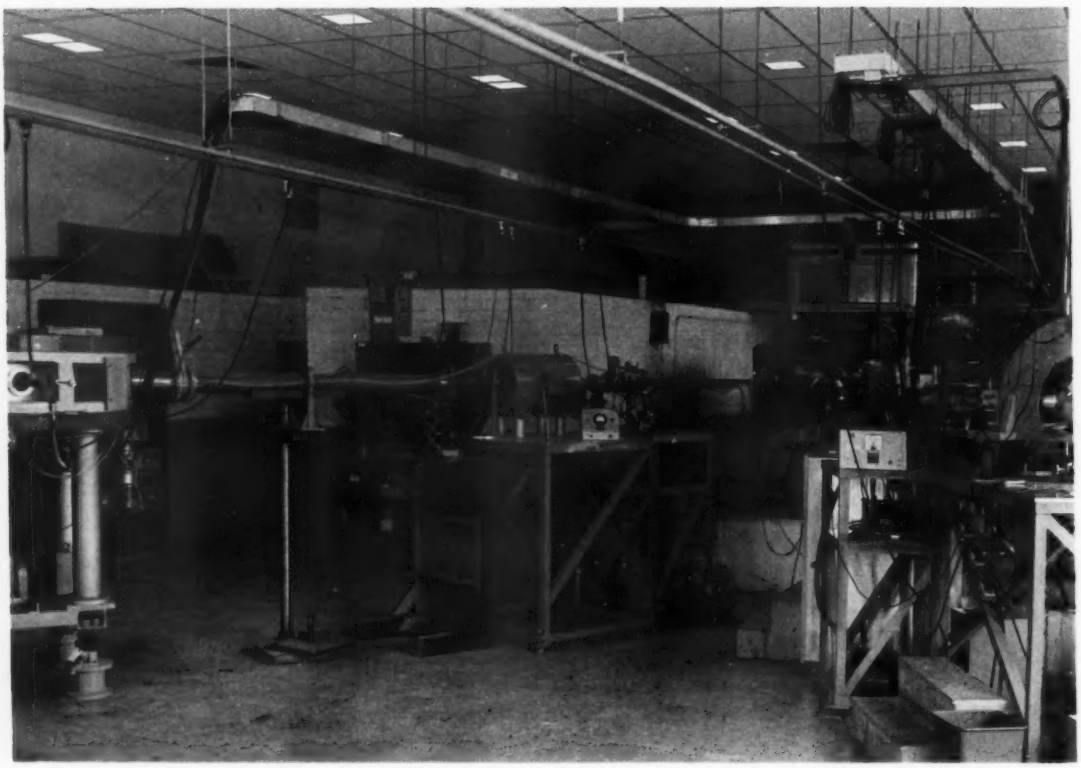
In each experiment, the computer-controlled system scans and reads the outputs from a predetermined number of sensors (measuring wind, temperature, etc.) located on a 100-foot tower, edits and processes the data, and records the results on magnetic tape. A printed real-time display of some of the important statistical parameters is also provided to keep the operator up-to-date on the state of the atmosphere. The system is capable of sampling sensor signals at rates up to 50 times a second, which is faster than the normal requirement for turbulence analysis. ★

Close-up of tower at site

ARL's 2-MeV Van de Graaff Accelerator

An important part of the fundamental knowledge of the structure of matter is that which pertains to the structure of the atomic nucleus. In turn, progress in fundamental understanding of nuclear structure and the basic nuclear forces depends in a critical manner upon the availability of experimental data on such nuclear properties as the energy, total angular momentum, parity, lifetime (or width), and decay properties of excited quantum states. These and other related data on nuclear parameters, when considered in relation to firmly established physical laws, are leading to major advances in the difficult problem of the nature of the atomic nucleus.

The ARL Nuclear Structure Group (General Physics Research Laboratory) has been primarily engaged during the past year in the acquisition of detailed data of the type mentioned above for excited states of selected nuclei in the region between oxygen-16 and calcium-40 in the periodic table of elements. The principal tool in this investigation has been a 2-MeV Van de Graaff accelerator. During this period, the accelerator has been used to provide beams of protons and deuterons with which nuclear reactions were induced in the appropriate target materials. The radiations emitted from the target as a result of these nuclear reactions were detected and analyzed by means of large NaI(Tl) gamma-ray and solid-state charged particle detectors. Computer techniques were used, where possible, in the analysis and theoretical interpretation of data so obtained.



The 2-MeV Van de Graaff particle accelerator operated by ARL's General Physics Research Laboratory

Control panel and instrumentation consoles for the 2-MeV Van de Graaff particle accelerator

New OAR center of activities

THE ARCHITECTS BUILDING, NEW HOME OF HQ OAR AND AFOSR IN ARLINGTON, VIRGINIA.

Near the Virginia ends of Francis Scott Key Bridge and Theodore Roosevelt Bridge, the building overlooks the Iwo Jima Memorial in Arlington and is opposite Georgetown University across the Potomac.